

Process control—a new quality control option from Infrasoftware International

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Introduction

Infrasoftware International Inc. (ISI) has recently developed a new Windows-based front end program for use with its NIRS software, which has been developed for use by production operators who have little or no technical or laboratory experience. The package, named NIRQA, enables the operators to take responsibility for the product that they are making, thus reducing the need for a full time quality assurance laboratory.

The package is fully compatible with and supported by the ISI NIRS 1, 2 and 3 programs and requires configuration, monitoring and support by expertly trained analysts. However, once configured, line operators will be able to get good quality, validated results with which to control their process.

The program can be networked via Windows for Workgroups, and is configurable to meet many diverse applications, by using the standard Windows functions or the files generated by NIRS. Messages produced by the standard Windows dialogue boxes can be customised and translated into other languages via a resource editor provided with the Borland C++ and many other program development packages.

The power of the software is in the simplicity of the operator interface, coupled with the complexity of the background processing, which has been designed to make intelligent assessments of the raw data from the analyser, prior to giving the operator a result. The operator is largely unaware of this procedure.

All user configuration is via simple text (.INI) files, which are a standard feature of Windows. Once the system has been configured and installed, the operator is presented with a series of drop down menu options by which to select his sample. The first level of selection is "AREA" which allows the workstation to be divided into discrete working areas, thus separating different departments that have access to the same instrument. The second level of selection defines the sample type and selects the calibration to be used. The first and second levels are mandatory, the third and fourth levels are optional and are descriptors which can be used to separate different sets of samples which may share a common calibration. At all times the operator is given instruction or information on the bottom line of the screen.

After selecting the sample type, the operator is asked to confirm his choice, enter some notes (optional) and is given a sample number. (There are currently two options of sample number format, others are available on request to ISI, these are configured via standard Windows .DLL files.) At this point, the operator has the opportunity to cancel and return to the beginning, review the last twenty analyses of this sample type or carry out an analysis. The display from the last twenty option is identical to the results display and will be described later. Drivers are currently available for the NIRSystems 6500 and the B+L (Technicon) models 400 and 450. There is also

a driver available for testing systems from spectral data stored on disk. Again these are configured using standard .DLL files and other options are available on request to ISI.

Once the computer system has received the raw data from the analyser, a spectrum of the sample may be displayed. This option is configurable, as the spectrum is not always useful (in the case of filter instruments) or desirable. At this point the operator can elect to continue or cancel. The raw data are then compared to a library set which should represent the range of samples designated as the “standard” product. If the sample matches this “target” library the software will then give the constituent results and, if desired, the “H” statistics for the sample. The library, principle component and equation files are developed using NIRS 2. The files are the same as those used in NIRS 1 and are totally interchangeable.

If the sample does not conform to the target library, the software will search other libraries and error files in an attempt to find a match. This is done in a structured fashion and is designed to give the operator as much information as possible. However, the system will not give a result if the sample does not conform to a standard set of samples. This effectively prevents the operator getting the wrong result.

The system can hold a large number of libraries. The “target” libraries are those with standard sample sets. There are also “default” libraries which have associated equation files designed to cover large general populations that include the target population as a discrete sub-population. If the sample does not conform to the sub-population, it may be covered by the larger general population and a result can then be given with confidence. The samples are designated with a flag “D” in the results screen. “Hidden” libraries are sets of samples which represent a known non-standard situation. If a process line is running outside its standard operating conditions due to a fault, this can be picked up and classified via principle components. If the problem reoccurs, the operator can be given the appropriate information. If a sample matches this type of library, a constituent result will not always be given. If a sample matches another library that is not a default or the designated target library, the result is flagged with “O” for “other” library. At this point if no match has been found, the system will evaluate the target library again and establish whether the sample is a near outlier of the sample set. The limits for this condition (known as high H or **) are set in the NIRS software in the PROD.SYS file for each product entry. If the sample conforms to this a result can be given from the target calibration but it is flagged as “H”.

A set of known errors may be stored in an error file. If all libraries have been searched and a match has not been found, this file is searched. These files should include situations such as no sample present, sample cup inserted upside down etc. Each set should be created in line with the applications installed at that workstation. To simplify the logic a simple flow diagram is given in Figure 1.

If the software is unable to find any matching conditions for the sample, the system has no alternative but to report that the sample cannot be identified. Unfortunately the operator is left without any information or results. The objective of the expert analysts and the system manager is to ensure that the system is educated with up-to-date information to prevent this situation occurring, by monitoring the calibrations, classifying non-conformance or error situations and adding them to the software.

After a successful analysis the results are displayed on a control chart, the limits of which are set by the experts. The current results, plus the results of the 19 most recent samples that match the current sample description, are displayed for each constituent. It is also possible to display the results of the principal components analysis (PCA) based “H” statistics (global and neighbourhood “H”) in this format. The system is set up, via *.INI files, to have a target value for each constituent (not to be confused with target libraries) with a range described as ± 2 standard deviations (SD). Any sample that falls within this limit is plotted in a green box on the graph at

Decisions made by NIRQA

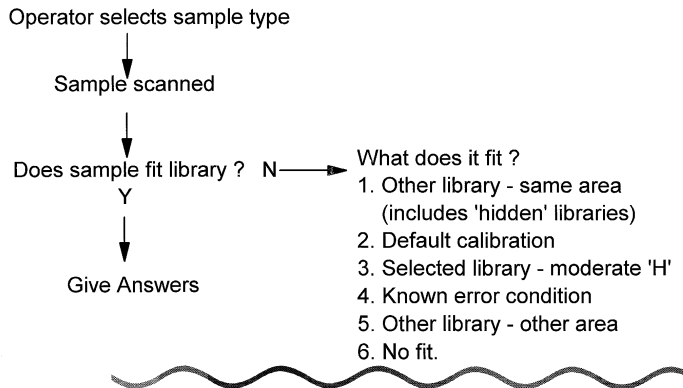


Figure 1. Schematic diagram of decisions made by NIRQA.

the appropriate position, along with any relevant flags. Further control limits are set at ± 3 SD. Samples with results falling between +2 and +3, or -2 and -3, SD are plotted in a yellow box with any appropriate flags. These yellow areas are designated warning areas where the operator should be aware that his process is out of control. Results that are less than 3 SD below the target or greater than 3 SD above the target are plotted in red. This area is designated as the action area and any samples falling in this area should have the appropriate positive action taken. As these targets and standard deviations are set by the expert users, it is possible to set the limits to reflect the capability of the process and each sample type can have its own limits applied. This information is also displayed when the operator selects the last twenty option from the confirmation screen. A tabular list of this information is available on selecting a button.

The operator can request a printout of the results and/or the last twenty screen and tabular list. On selection of the OK button from the results screen the operator is returned to the start to select a new sample.

In order to run cross-check samples on a “live” system without affecting the operators trend charts, an expert user can switch to “privileged operator mode” via a user definable hot key. In this mode, all data are stored in a separate directory for use in calibration development and monitoring. It is also possible to install new analysis options for use only in privileged operator mode, which are not available to line operators.

The system stores ALL raw data. Any which have matched a library are stored in the product's file. Any which have failed to match a library are stored in an IDFAIL file. Predicted results are also stored where available. All of this data can also be stored on up to two other disk drives in the networked workgroup from operator mode and one other disk drive in the workgroup from privileged operator mode. This is done at the time of each analysis and provides the ultimate “mirror” back up. When any raw or predicted data file reaches a user defined limit (defaulted to 2047) all data up to the last 47 results are copied out to an archive file, leaving the last set of results for continuity of the trend charts. The archive file is given a unique file name based on the original and is stored only on the remote drives.

Data can be output to an ASCII file for transmission to other computer systems. This file is user configurable and is formatted simply in a text file, using the same method as the results printouts from NIRS (form.out).

The software also includes a laboratory information management system (LIMS) mode. If an incoming raw material requires near infrared (NIR) checks the sample information is automatically sent from the LIMS system to the appropriate NIR workstation as the sample is logged in and NIRQA builds a worklist for the operator to select from. On completion of the analysis, the results are automatically posted back to the LIMS system. Each LIMS system will have to be configured individually, the option currently available is for the Beckman Labmanager system.

Conclusion

This description of NIRQA gives only a cursory view of the software. In order to see the full benefits a demonstration of the package is recommended.